Full wwPDB EM Validation Report

May 16, 2024 – 09:50 am BST

PDB ID	:	6YW7
EMDB ID	:	EMD-10960
Title	:	Cryo-EM structure of the ARP2/3 1A5C isoform complex.
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Deposited on	:	2020-04-29
Resolution	:	4.50 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 Å.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5426 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Actin-related protein 3.

Mol	Chain	Residues	Atoms			AltConf	Trace
1	A	396	Total 1188	C 792	N 396	0	0

- Molecule 2 is a protein called Actin-related protein 2/3 complex subunit 2.

Mol	Chain	Residues	Atoms			AltConf	Trace
2	D	284	Total 852	C 568	N 284	0	0

- Molecule 3 is a protein called Actin-related protein 2/3 complex subunit 3.

Mol	Chain	Residues	Atoms			AltConf	Trace
3	E	170	Total 510	C 340	N 170	0	0

- Molecule 4 is a protein called Actin-related protein 2.

Mol	Chain	Residues	Atoms			AltConf	Trace
4	B	286	Total 858	C 572	N 286	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	35	ILE	LEU	conflict	UNP P61160

- Molecule 5 is a protein called Actin-related protein 2/3 complex subunit 4.

Mol	Chain	Residues	Atoms			AltConf	Trace
5	F	165	Total 495	C 330	N 165	0	0

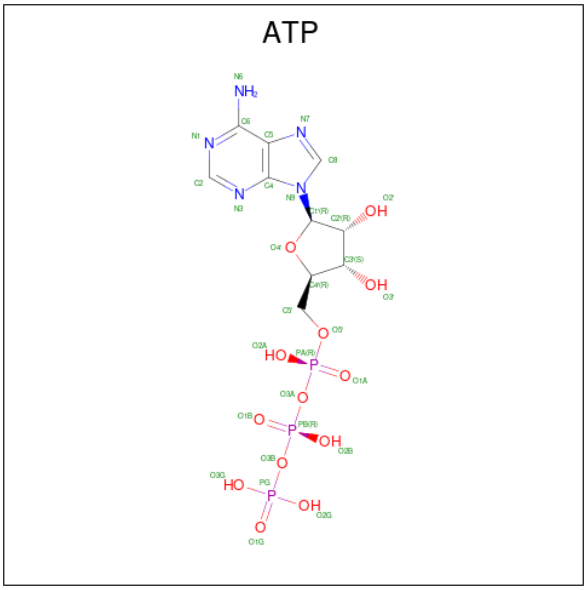
- Molecule 6 is a protein called Actin-related protein 2/3 complex subunit 5.

Mol	Chain	Residues	Atoms			AltConf	Trace
6	G	139	Total	C	N	0	0
			417	278	139		

- Molecule 7 is a protein called Actin-related protein 2/3 complex subunit 1A.

Mol	Chain	Residues	Atoms			AltConf	Trace
7	C	348	Total	C	N	0	0
			1044	696	348		

- Molecule 8 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
8	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

MolProbity failed to run properly - this section is therefore empty.

3 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	130973	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	59	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	ATP	B	401	-	26,33,33	0.92	1 (3%)	31,52,52	1.43	4 (12%)
8	ATP	A	501	-	26,33,33	0.90	1 (3%)	31,52,52	1.67	6 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ATP	B	401	-	-	7/18/38/38	0/3/3/3
8	ATP	A	501	-	-	2/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	401	ATP	C5-C4	2.37	1.47	1.40
8	A	501	ATP	C5-C4	2.31	1.47	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	501	ATP	PA-O3A-PB	-3.89	119.47	132.83
8	A	501	ATP	C1'-N9-C4	-3.74	120.07	126.64
8	B	401	ATP	PA-O3A-PB	-3.60	120.47	132.83
8	A	501	ATP	C4-C5-N7	-3.25	106.01	109.40
8	A	501	ATP	N3-C2-N1	-3.23	123.63	128.68
8	B	401	ATP	N3-C2-N1	-3.14	123.78	128.68
8	A	501	ATP	C3'-C2'-C1'	3.08	105.61	100.98
8	B	401	ATP	C3'-C2'-C1'	3.05	105.58	100.98
8	B	401	ATP	C4-C5-N7	-2.75	106.53	109.40
8	A	501	ATP	PB-O3B-PG	-2.61	123.88	132.83

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	401	ATP	PB-O3B-PG-O2G

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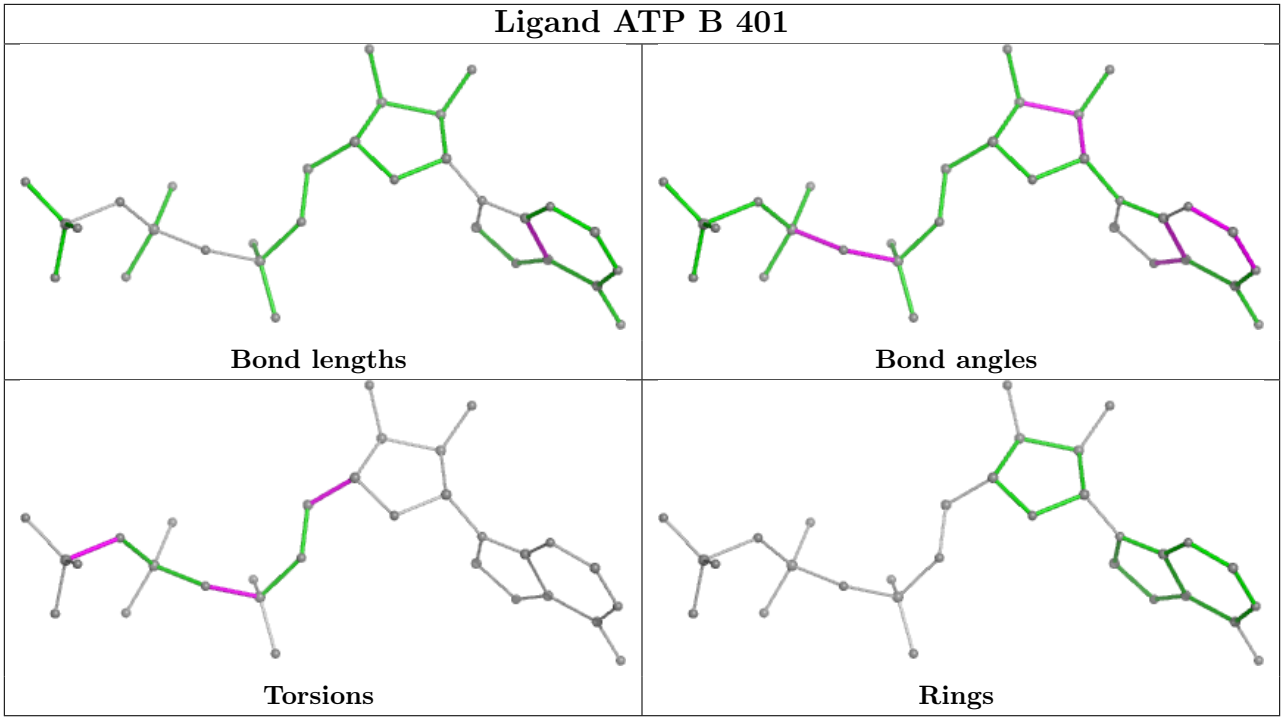
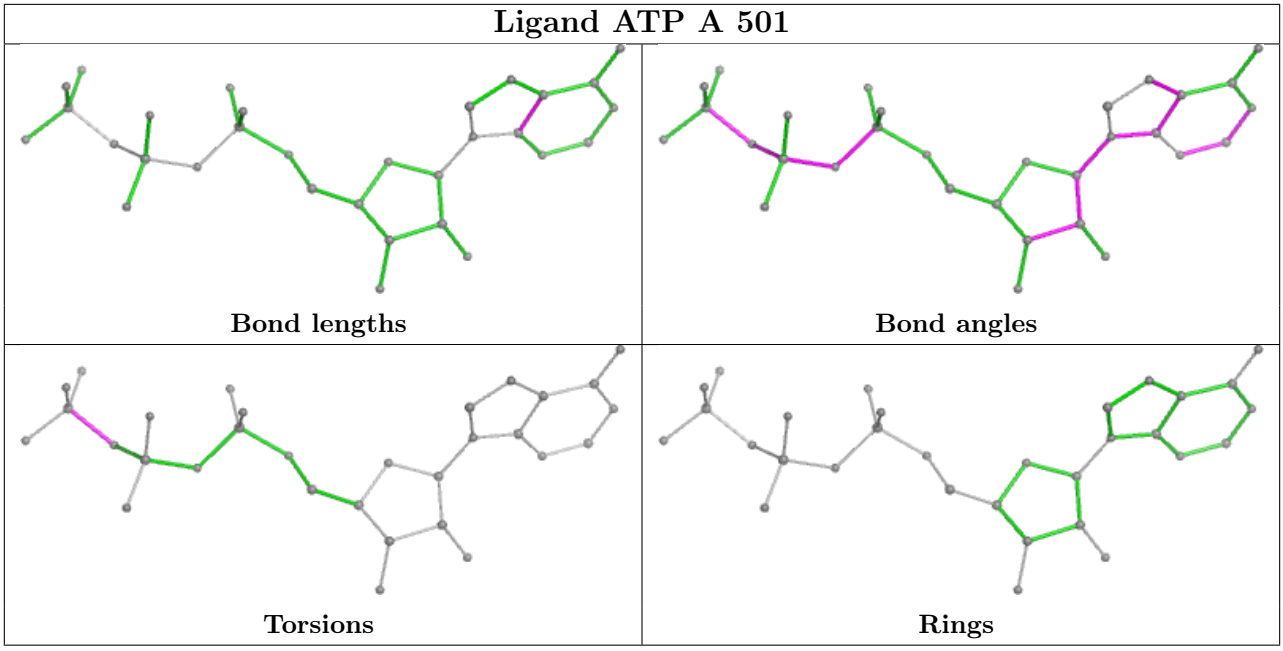
Mol	Chain	Res	Type	Atoms
8	B	401	ATP	C3'-C4'-C5'-O5'
8	B	401	ATP	O4'-C4'-C5'-O5'
8	B	401	ATP	PB-O3A-PA-O2A
8	A	501	ATP	PB-O3B-PG-O3G
8	B	401	ATP	PB-O3B-PG-O3G
8	B	401	ATP	PB-O3A-PA-O1A
8	A	501	ATP	PB-O3B-PG-O1G
8	B	401	ATP	PB-O3B-PG-O1G

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3
3	E	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	105:ILE	C	106:PRO	N	4.37
1	A	83:VAL	C	84:GLU	N	1.73
1	E	34:ARG	C	35:GLU	N	1.20
1	A	63:GLY	C	64:ASP	N	1.19
1	A	280:GLU	C	281:ILE	N	1.15

5 Map visualisation

This section contains visualisations of the EMDB entry EMD-10960. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

5.1 Orthogonal projections

This section was not generated.

5.2 Central slices

This section was not generated.

5.3 Largest variance slices

This section was not generated.

5.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

5.5 Orthogonal surface views

This section was not generated.

5.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

6 Map analysis

This section contains the results of statistical analysis of the map.

6.1 Map-value distribution

This section was not generated.

6.2 Volume estimate versus contour level

This section was not generated.

6.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

7 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

8 Map-model fit

This section was not generated.